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Lattice vibrations of layer structures

PRADIP N. GHOSH

Department of Physics, University of Calcutta, Calcutta 700009

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Layered crystals of cadmium-chloride type are used as hosts for studying Jahn-Teller effects (Freeman & Jones 1969) of many transition metal ions. In solids, this effect arises from vibronic coupling of the orbitally degenerate electronic states of the ions with the lattice vibrations of the host structure. This has revived interest in the dynamics of the layer structures. Very recently, from Raman and infrared spectroscopic investigation Lockwood (1973) has reported the commanding role of the layer like nature in the lattice vibrations of cadmium chloride, cadmium bromide, manganese chloride and cobalt chloride structures. The present work is a preliminary report on a linear chain model used to interpret the long wave length lattice vibrations of the layer structures.

$CdCl_2$-type crystals (Lockwood 1969) are composed of triplanar layers in the sense that each layer consists of three parallel planes—a cation plane with two anion planes on either side of it. These layers are then held together by weak Van der Waals froces. There is a single layer per primitive unit cell. A factor group analysis with D_{3d} character table shows that there are four optical modes of vibration ($A_{1g}+A_{2u}+E_g+E_u$) and two acoustic modes ($A_{2u}+E_u$). In a linear chain model we have used only nearest neighbour intralayer force constants K_c and K_s corresponding to compressional and shear motions of the planes respectively. The parallel planes are perpendicular to the linear chain. Frequencies ($\boldsymbol{K} = 0$) are obtained as given by

optical $$\omega^2(A_{1g}, E_g) = \frac{K}{m}, \qquad \ldots (1)$$

acoustic $$\omega^2(A_{2u}, E_u) = 0, \qquad \ldots (2)$$

optical $$\omega^2(A_{2u}, E_u) = K\left(\frac{1}{m}+\frac{3}{4}\frac{1}{M}\mp\frac{1}{\sqrt{mM}}\right), \qquad \ldots (3)$$

where m and M are masses of halogen and metal atoms respectively. In formulae (1) and (3) K is either K_C or K_S for compressional (A_{1g}, A_{2u}) or shear (E_g, E_u) motions as the case may be; the negative and positive signs correspond to A_{2u} and E_u modes respectively in formula (3). In table 1 we list the calculated and experimental frequencies for the four structures.

Table 1. Calculated and experimental frequencies for first order $K = 0$ phonons

Structure	Frequencies in cm^{-1}							
	A_{1g}(a)		A_{2u}		E_g(a)		E_u	
	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.
$CdCl_2$	233	233	190	164	131	131	176	210
$CdBr_2$	148	148	123	102	77	77	119	161
$MnCl_2$	234	234	193	180	144	144	218	230
$CoCl_2$	250	250	205	190	152	152	227	235

(a) Frequencies for A_{1g} and E_g modes are used in obtaining force constants.

Data in table 1 show that the model (with neglect of interlayer force constants) works well for the layer structures. The relatively large error in case of $CdCl_2$ and $CdBr_2$ compared to $MnCl_2$ and $CoCl_2$ may be due to long range ionic forces as the bonds Cd–Cl and Cd–Br are more ionic in nature. In these cases nearest neighbour approximation cannot be expected to give accurate result, effect of the interactions with more distant neighbours is being studied at present and will be communicated shortly.

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Physical aspect of fine spinning of jute

N. G. Sinha

Jute Technological Research Laboratories, I.C.A.R.,
12, *Regent Park, Calcutta*-700040

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Jute is a multicellular fibre of meshy structure. The number of cells varies from 3 to 20 in a fibre entity. The fineness of fibres varies from 1.20 to 5.00 tex, i.e., about 5 to 20 times coarser than cotton which has a single cell. The jute fibre is